## Bell Inequalities Classifying Bi-separable Three-qubit States

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## Abstract

We present a set of Bell inequalities that gives rise to a finer classification of the entanglement for tripartite systems. These inequalities distinguish three possible bi-separable entanglements for three-qubit states. The three Bell operators we employed constitute an external sphere of the separable cube.

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The Bell inequality [1] provided the first possibility to distinguish experimentally between quantum-mechanical predictions and those of local realistic models. Since Bell's work, there were many important generalizations [2, 3, 4, 5]. We refer to [6] and references therein as recent nice reviews.

The inequalities in [7, 8] can lead to a detailed classification of multipartite entanglement. By generalizing the method used in [10], where Bell inequalities that violate the generalized GHZ state and involve only two measurement settings per observer are investigated, in this letter we present a set of Bell inequalities that gives rise to a finer classification of the entanglement for tripartite systems. In classifying bi-separable three-qubit states, these inequalities determine further which qubit is separated from the rest two. Moreover it is shown that the three Bell operators we employed constitute a sphere. The detailed classifications are depicted according to parameter regions in the sphere.

Consider N parties and allow each of them to choose independently between two dichotomic observables  $A_j$ ,  $B_j$  for the j-th observer, where  $A_j = \vec{a}_j \cdot \vec{\sigma}^j$  and  $B_j = \vec{b}_j \cdot \vec{\sigma}^j$ , with  $\vec{\sigma}^j = (\sigma_1^j, \sigma_2^j, \sigma_3^j)$  the Pauli matrices on the j-th qubit, and  $\vec{a}_j = (a_j^1, a_j^2, a_j^3)$ ,  $\vec{b}_j = (b_j^1, b_j^2, b_j^3)$  the real unit vectors. We define

$$\mathcal{D}_N^{(i)} = \mathcal{B}_{N-1}^{(i)} \otimes \frac{1}{2} (A_i + B_i) + \frac{1}{2} (A_i - B_i), \ i = 1, \dots, N,$$
 (1)

where  $\mathcal{B}_{N-1}^{(i)}$  is the quantum mechanical Bell operator of WWZB inequalities [3, 4] on the N-1 qubits except for the *i*-th qubit.

For tripartite case (N=3), for example, we have  $\mathcal{B}_2^{(2)} = \frac{1}{2}(A_1B_3 + B_1A_3 + A_1A_3 - B_1B_3)$ , and

$$\mathcal{D}_{3}^{(2)} = \mathcal{B}_{2}^{(2)} \otimes \frac{1}{2} (A_{2} + B_{2}) + \frac{1}{2} (A_{2} - B_{2})$$

$$= \frac{1}{4} (A_{1} (A_{2} + B_{2}) A_{3} + A_{1} (A_{2} + B_{2}) B_{3} + B_{1} (A_{2} + B_{2}) A_{3} - B_{1} (A_{2} + B_{2}) B_{3})$$

$$+ I \otimes \frac{1}{2} (A_{2} - B_{2}) \otimes I.$$

It is straightforward to prove that for fully separable states  $\rho$ , the average values  $\langle \mathcal{D}_3^{(i)} \rangle_{\rho}$  of  $\mathcal{D}_3^{(i)}$  satisfy  $|\langle \mathcal{D}_3^{(i)} \rangle_{\rho}| \leq 1$  for i = 1, 2, 3.

Let  $S_{1-23}$ ,  $S_{2-13}$  and  $S_{12-3}$  denote the bi-separable states of the form  $\rho_1 \otimes \rho_{23}$ ,  $\rho_2 \otimes \rho_{13}$ , and  $\rho_{12} \otimes \rho_3$  respectively. We have

[Theorem 1] For states  $\rho$  in  $S_{1-23}$ ,  $S_{2-13}$  and  $S_{12-3}$ , respectively we have:

$$|\langle \mathcal{D}_3^{(1)} \rangle_{\rho}| \le \sqrt{2}, \quad |\langle \mathcal{D}_3^{(2)} \rangle_{\rho}| \le 1, \quad |\langle \mathcal{D}_3^{(3)} \rangle_{\rho}| \le 1, \tag{2}$$

$$|\langle \mathcal{D}_3^{(1)} \rangle_{\rho}| \le 1, \quad |\langle \mathcal{D}_3^{(2)} \rangle_{\rho}| \le \sqrt{2}, \quad |\langle \mathcal{D}_3^{(3)} \rangle_{\rho}| \le 1 \tag{3}$$

and

$$\left| \langle \mathcal{D}_3^{(1)} \rangle_{\rho} \right| \le 1, \quad \left| \langle \mathcal{D}_3^{(2)} \rangle_{\rho} \right| \le 1, \quad \left| \langle \mathcal{D}_3^{(3)} \rangle_{\rho} \right| \le \sqrt{2}. \tag{4}$$

[Proof] That  $|\langle \mathcal{D}_3^{(i)} \rangle_{\rho}|$  has the bound  $\sqrt{2}$  for all 3-qubit states can be seen from  $\langle \mathcal{D}_3^{(1)} \rangle^2 = \frac{1}{2}(1+\vec{a}_1 \cdot \vec{b}_1)\langle \mathcal{B}_3^{(1)} \rangle^2 + \frac{1}{2}(1-\vec{a}_1 \cdot \vec{b}_1) \leq 2$ , taking into account the result  $\langle \mathcal{B}_3^{(1)} \rangle^2 \leq 2$  in [3]. As an example we consider the states in  $S_{12-3}$  and prove the inequalities in (4) in the following. Due to the linear property of average values, we only need to discuss pure states. From the Schmidt biorthogonal decomposition theorem [11], every pure state in  $S_{12-3}$  can be written as

$$|\psi\rangle = (\cos\alpha|01\rangle - \sin\alpha|10\rangle) \otimes |0\rangle \equiv |\psi\rangle_{12} \otimes |\psi\rangle_{3}. \tag{5}$$

Therefore

$$\begin{split} & |\langle \mathcal{D}_{3}^{(1)} \rangle_{|\psi\rangle}| \\ &= |\langle \frac{A_{1} + B_{1}}{2} \frac{A_{2} + B_{2}}{2} \rangle_{|\psi\rangle_{12}} \langle A_{3} \rangle_{|\psi\rangle_{3}} + \langle \frac{A_{1} + B_{1}}{2} \frac{A_{2} - B_{2}}{2} \rangle_{|\psi\rangle_{12}} \langle B_{3} \rangle_{|\psi\rangle_{3}} + \langle \frac{A_{1} - B_{1}}{2} \rangle_{|\psi\rangle}| \\ &\leq \sup |\langle \frac{A_{1} + B_{1}}{2} \frac{A_{2} + B_{2}}{2} \rangle_{|\psi\rangle_{12}} + \langle \frac{A_{1} + B_{1}}{2} \frac{A_{2} - B_{2}}{2} \rangle_{|\psi\rangle_{12}} + \langle \frac{A_{1} - B_{1}}{2} \rangle_{|\psi\rangle}| \\ &= \sup |\langle \frac{A_{1} + B_{1}}{2} A_{2} \rangle_{|\psi\rangle_{12}} + \langle \frac{A_{1} - B_{1}}{2} \rangle_{|\psi\rangle}| \\ &= \frac{1}{2} \sup |(a_{1}^{3} + b_{1}^{3}) a_{2}^{3} + \sin 2\alpha ((a_{1}^{1} + b_{1}^{1}) a_{2}^{1} + (a_{1}^{2} + b_{1}^{2}) a_{2}^{2}) + \cos 2\alpha (a_{1}^{3} - b_{1}^{3})|. \end{split}$$

The maximum is obtained at either  $\alpha = 0$  or  $\alpha = \frac{\pi}{4}$ . For the case  $\alpha = 0$  the state (5) is factorizable and the inequality is trivially satisfied. For the case  $\alpha = \frac{\pi}{4}$  we have

$$|\langle \mathcal{D}_3^{(1)} \rangle_{|\psi\rangle}| \le \sup \frac{1}{2} |(\vec{a}_1 + \vec{b}_1) \cdot \vec{a}_2| = 1.$$

Similarly we can prove  $|\langle \mathcal{D}_3^{(2)} \rangle_{|\psi\rangle}| \leq 1$ . The inequalities in (2) and (3) can be also proved accordingly.

If we consider  $\langle \mathcal{D}_3^{(i)} \rangle_{\rho}$ , i=1,2,3 to be three coordinates, then all the fully separable states are confined in a cube with size  $2 \times 2 \times 2$ . While from the Theorem 1, the bi-separable states are in a cuboid with the size either  $2\sqrt{2} \times 2 \times 2$  or  $2 \times 2\sqrt{2} \times 2$  or  $2 \times 2 \times 2\sqrt{2}$ , which correspond to three bi-separable cases:  $S_{1-23}$ ,  $S_{2-13}$  and  $S_{12-3}$ . The states in other regions are then tripartite entangled. However there exists a quadratic inequality that strengthens the range.

[Theorem 2] For all 3-qubit states, we have the following inequality:

$$\langle \mathcal{D}_3^{(1)} \rangle_\rho^2 + \langle \mathcal{D}_3^{(2)} \rangle_\rho^2 + \langle \mathcal{D}_3^{(3)} \rangle_\rho^2 \le 3. \tag{6}$$

[Proof] A 3-qubit state  $\rho$  can be generally expressed as [9]:

$$\rho = \frac{1}{8} (I + \alpha_i \sigma_i^1 + \beta_i \sigma_i^2 + \gamma_i \sigma_i^3 + R_{ij} \sigma_i^1 \sigma_j^2 + S_{ij} \sigma_i^1 \sigma_j^3 + T_{ij} \sigma_i^2 \sigma_j^3 + Q_{ijk} \sigma_i^1 \sigma_j^2 \sigma_k^3), \tag{7}$$

where  $\sigma_i^j$  are the *i*-th Pauli matrices on the *j*-th qubit, e.g.  $\sigma_i^1 = \sigma_i \otimes I \otimes I$ ,  $\alpha_i$ ,  $\beta_i$ ,  $\gamma_i$ ,  $R_{ij}$ ,  $S_{ij}$ ,  $T_{ij}$  and  $Q_{ijk}$  are some real coefficients. The repeated indices are assumed to be summed over from 1 to 3. As the expression  $\omega = \langle \mathcal{D}_3^{(1)} \rangle_{\rho}^2 + \langle \mathcal{D}_3^{(2)} \rangle_{\rho}^2 + \langle \mathcal{D}_3^{(3)} \rangle_{\rho}^2$  is a convex function of  $\rho$ , it is sufficient to consider pure states only. Let  $\rho = |\Psi\rangle\langle\Psi|$ . For three qubits states,  $|\Psi\rangle$  has the following decomposition [12]:

$$|\Psi\rangle = l_0|000\rangle + l_1 e^{i\phi}|100\rangle + l_2|101\rangle + l_3|110\rangle + l_4|111\rangle,$$
 (8)

with normalization condition

$$0 \le \phi \le \pi$$
,  $\lambda_i \ge 0$ ,  $\sum_i \lambda_i^2 = 1$ ,  $i = 1, ..., 4$ .

Comparing  $\rho = |\Psi\rangle\langle\Psi|$  with the general expression (7), we have the following relations after some straightforward calculations,

$$\sum_{i,j=1}^{3} (R_{ij}^2 + S_{ij}^2 + T_{ij}^2) = 3, \quad \sum_{i,j,k=1}^{3} Q_{ijk}^2 + \sum_{i=1}^{3} (\alpha_i^2 + \beta_i^2 + \gamma_i^2) = 4.$$

As  $\sum \alpha_i^2$ ,  $\sum R_{ij}^2$ ,  $\sum Q_{ijk}^2$  etc. are all invariants under local unitary transformations [9], the relations above hold not only for state (8), but also for all pure states. We simply denote these relations as  $|\vec{R}|^2 + |\vec{S}|^2 + |\vec{T}|^2 = 3$ ,  $|\vec{Q}|^2 + |\vec{\alpha}|^2 + |\vec{\beta}|^2 + |\vec{\gamma}|^2 = 4$ . Because  $|\vec{\alpha}|$ ,  $|\vec{\beta}|$ ,  $|\vec{\gamma}| \leq 1$ , we have  $1 \leq |\vec{Q}| \leq 2$ . The minimum is attained when  $|\Psi\rangle$  is fully separable and the maximum is obtained for the maximally entangled state, i.e. the GHZ state.

Set  $C_i = \frac{1}{2}(A_i + B_i)$ ,  $D_i = \frac{1}{2}(A_i - B_i)$  and  $\vec{s}_i = \frac{1}{2}(\vec{a}_i + \vec{b}_i)$ ,  $\vec{t}_i = \frac{1}{2}(\vec{a}_i - \vec{b}_i)$ , for i = 1, 2, 3. We have  $|\vec{s}_i|^2 + |\vec{t}_i|^2 = 1$  and  $\vec{s}_i \cdot \vec{t}_i = 0$ . The operators  $\mathcal{D}_3^{(i)}$  can be rewritten as:

$$\mathcal{D}_3^{(1)} = C_1 C_2 C_3 + C_1 C_2 D_3 + C_1 D_2 C_3 - C_1 D_2 D_3 + D_1,$$

$$\mathcal{D}_3^{(2)} = C_1 C_2 C_3 + C_1 C_2 D_3 + D_1 C_2 C_3 - D_1 C_2 D_3 + D_2,$$

$$\mathcal{D}_3^{(3)} = C_1 C_2 C_3 + C_1 D_2 C_3 + D_1 C_2 C_3 - D_1 D_2 C_3 + D_3.$$

Then

$$\omega = \langle \Psi | \mathcal{D}_{3}^{(1)} | \Psi \rangle_{\rho}^{2} + \langle \Psi | \mathcal{D}_{3}^{(2)} | \Psi \rangle_{\rho}^{2} + \langle \Psi | \mathcal{D}_{3}^{(3)} | \Psi \rangle_{\rho}^{2}$$

$$= (\vec{s}_{1} \otimes \vec{s}_{2} \otimes \vec{s}_{3} \cdot \vec{Q} + \vec{s}_{1} \otimes \vec{s}_{2} \otimes \vec{t}_{3} \cdot \vec{Q} + \vec{s}_{1} \otimes \vec{t}_{2} \otimes \vec{s}_{3} \cdot \vec{Q} - \vec{s}_{1} \otimes \vec{t}_{2} \otimes \vec{t}_{3} \cdot \vec{Q} + \vec{t}_{1} \cdot \vec{\alpha})^{2}$$

$$+ (\vec{s}_{1} \otimes \vec{s}_{2} \otimes \vec{s}_{3} \cdot \vec{Q} + \vec{s}_{1} \otimes \vec{s}_{2} \otimes \vec{t}_{3} \cdot \vec{Q} + \vec{t}_{1} \otimes \vec{s}_{2} \otimes \vec{s}_{3} \cdot \vec{Q} - \vec{t}_{1} \otimes \vec{s}_{2} \otimes \vec{t}_{3} \cdot \vec{Q} + \vec{t}_{2} \cdot \vec{\beta})^{2}$$

$$+ (\vec{s}_{1} \otimes \vec{s}_{2} \otimes \vec{s}_{3} \cdot \vec{Q} + \vec{s}_{1} \otimes \vec{t}_{2} \otimes \vec{s}_{3} \cdot \vec{Q} + \vec{t}_{1} \otimes \vec{s}_{2} \otimes \vec{s}_{3} \cdot \vec{Q} - \vec{t}_{1} \otimes \vec{t}_{2} \otimes \vec{s}_{3} \cdot \vec{Q} + \vec{t}_{3} \cdot \vec{\gamma})^{2},$$

where  $\vec{s} \otimes \vec{t} \otimes \vec{p} \cdot \vec{Q}$  stands for  $\sum_{ijk} s_i t_j p_k Q_{ijk}$ . From this expression, we see that  $\omega$  attains its maximum at either  $|\vec{Q}| = 1$  or  $|\vec{Q}| = 2$ . For the case  $|\vec{Q}| = 1$ , the state  $|\Psi\rangle$  is fully separable and the inequality is trivially satisfied. In the second case  $|\vec{Q}| = 2$  we have:

$$\omega = (\vec{s}_1 \otimes \vec{s}_2 \otimes \vec{s}_3 \cdot \vec{Q} + \vec{s}_1 \otimes \vec{s}_2 \otimes \vec{t}_3 \cdot \vec{Q} + \vec{s}_1 \otimes \vec{t}_2 \otimes \vec{s}_3 \cdot \vec{Q} - \vec{s}_1 \otimes \vec{t}_2 \otimes \vec{t}_3 \cdot \vec{Q})^2$$

$$+ (\vec{s}_1 \otimes \vec{s}_2 \otimes \vec{s}_3 \cdot \vec{Q} + \vec{s}_1 \otimes \vec{s}_2 \otimes \vec{t}_3 \cdot \vec{Q} + \vec{t}_1 \otimes \vec{s}_2 \otimes \vec{s}_3 \cdot \vec{Q} - \vec{t}_1 \otimes \vec{s}_2 \otimes \vec{t}_3 \cdot \vec{Q})^2$$

$$+ (\vec{s}_1 \otimes \vec{s}_2 \otimes \vec{s}_3 \cdot \vec{Q} + \vec{s}_1 \otimes \vec{t}_2 \otimes \vec{s}_3 \cdot \vec{Q} + \vec{t}_1 \otimes \vec{s}_2 \otimes \vec{s}_3 \cdot \vec{Q} - \vec{t}_1 \otimes \vec{t}_2 \otimes \vec{s}_3 \cdot \vec{Q})^2$$

Without losing generality, we consider the maximally entangled state  $|\Psi\rangle$  of the form  $|\Psi\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ . We have then  $Q_{ijk} = 0$  except for  $Q_{111} = 1$ ,  $Q_{122} = Q_{212} = Q_{221} = -1$ . To attain the maximum of  $\omega$ , the third components of  $\vec{s}_i$ ,  $\vec{t}_i$  should be zero, and either  $|\vec{s}_i| = |\vec{t}_i|$  or one of the  $|\vec{s}_i|$  and  $|\vec{t}_i|$  is zero and the other one is 1. We deal with these cases respectively.

(1) The cases 
$$|\vec{s}_i| = 1$$
,  $|\vec{t}_i| = 0$ ,  $i = 1, 2, 3$ , 
$$\omega = 3(\vec{s}_1 \otimes \vec{s}_2 \otimes \vec{s}_3 \cdot \vec{Q})^2 = 3\langle \Psi | C_1 C_2 C_3 | \Psi \rangle^2 \leq 3.$$

(2) Cases of the form 
$$|\vec{s}_1| = |\vec{s}_2| = 1$$
 ( $|\vec{t}_1| = |\vec{t}_2| = 0$ ) and  $|\vec{s}_3| = |\vec{t}_3| = \frac{1}{\sqrt{2}}$ , then 
$$\omega = 2(\vec{s}_1 \otimes \vec{s}_2 \otimes \vec{s}_3 \cdot \vec{Q} + \vec{s}_1 \otimes \vec{s}_2 \otimes \vec{t}_3 \cdot \vec{Q})^2 + (\vec{s}_1 \otimes \vec{s}_2 \otimes \vec{s}_3 \cdot \vec{Q})^2$$
$$= 2\langle \Psi | C_1 C_2 (C_3 + D_3) | \Psi \rangle^2 + \langle \Psi | C_1 C_2 C_3 | \Psi \rangle^2 \leq 3.$$

(3) Cases like  $|\vec{s}_1| = 1$  ( $|\vec{t}_1| = 0$ ) and  $|\vec{s}_i| = |\vec{t}_i| = \frac{1}{\sqrt{2}}$  for i = 2, 3. From the orthogonal relation of  $\vec{s}_i$  and  $\vec{t}_i$ , we can express them as:  $\vec{s}_1 = (\cos\theta_1, \sin\theta_1, 0)$  and  $\vec{s}_i = \frac{1}{\sqrt{2}}(\cos\theta_i, \sin\theta_i, 0)$ ,  $\vec{t}_i = \frac{1}{\sqrt{2}}(-\sin\theta_i, \cos\theta_i, 0)$ , for i = 2, 3. Direct calculations lead to

$$\omega = \frac{3}{2}(\cos(\theta_1 + \theta_2 + \theta_3) - \sin(\theta_1 + \theta_2 + \theta_3))^2 \le 3.$$
 (9)

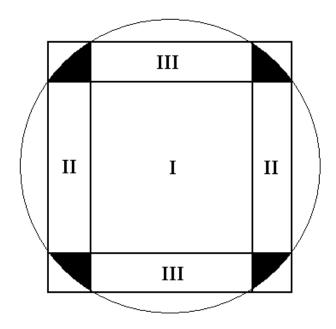


FIG. 1: Projection of the sphere related to the space of three-qubit entanglement

(4)  $|\vec{s}_i| = |\vec{t}_i| = \frac{1}{\sqrt{2}}$ . Set  $\vec{s}_i = \frac{1}{\sqrt{2}}(\cos\theta_i, \sin\theta_i, 0)$ ,  $\vec{t}_i = \frac{1}{\sqrt{2}}(-\sin\theta_i, \cos\theta_i, 0)$ , for i = 1, 2, 3. We get the same result as (9).

This ends the proof.  $\Box$ 

By regarding the average of  $\mathcal{D}_3^{(1)}$ ,  $\mathcal{D}_3^{(2)}$ ,  $\mathcal{D}_3^{(3)}$  as three axes of the space, we have that all the 3-qubit states are in the cube of edge length  $2\sqrt{2}$  with the center at the origin. But the inequality in Theorem 2 restricts all the states into a ball with radius  $\sqrt{3}$  centered at the origin, which is just the external ball of the cube of edge length 2. Therefore all the states are located in the common space of the larger cube of edge length  $2\sqrt{2}$  and the ball with radius  $\sqrt{3}$ , where the smaller cube of edge length 2 is for separable states, and the rest space is for all kinds of entangled states.

If we project the state space along the direction  $\mathcal{D}_3^{(3)}$  to the plane  $(\mathcal{D}_3^{(1)}, \mathcal{D}_3^{(2)})$  (cut the sphere in the  $(\mathcal{D}_3^{(1)}, \mathcal{D}_3^{(2)})$  plane), we get the Figure 1. The completely separable states are in the region labeled I, the left and right rectangular regions labeled II belong to  $S_{1-23}$ , and the top and bottom rectangular regions III belong to  $S_{2-13}$  (the states in  $S_{12-3}$  are in front of and behind the region I which could not be seen due to projection). The rest entangled states are located in the (corners) black regions.

We have presented a set of Bell inequalities which distinguish three possible bi-separable entanglements of tripartite qubit systems. The three Bell operators we used constitute an external sphere of the separable cube. By using the Bell operators defined in (1), the results can be generalized to N-qubit system. We conjecture that, for N-qubit system, one would have

$$\sum_{i=1}^{N} \langle \mathcal{D}_{N}^{(i)} \rangle_{\rho}^{2} \leq N.$$

Nevertheless, the generalized Bell quantities would only detect the entanglement between one qubit and the rest ones. For instance, for four-qubit systems, one can only learn from  $|\langle \mathcal{D}_4^{(1)} \rangle| > 1$  that the first qubit is entangled with the rest three qubits. One needs more Bell operators to classify all other possible entanglements.

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